

2,3,4-Trinitrotoluene  
602-29-9 | DTXSID60208944

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 8.49e-12 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 1.64e-01

**Confidence level:** 5.41e-01

## Nearest Neighbors from the Training Set

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2-Methyl-p-benzoquinone

**Measured:** 2.35e-11

**Predicted:** 2.15e-11

Image not found

1,4-Naphthoquinone

**Measured:** 3.10e-12

**Predicted:** 3.16e-11

Image not found

1,4-Benzoquinone

**Measured:** 4.60e-12

**Predicted:** 5.97e-12

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2,5-Furandione

**Measured:** 1.45e-12

**Predicted:** 2.17e-12